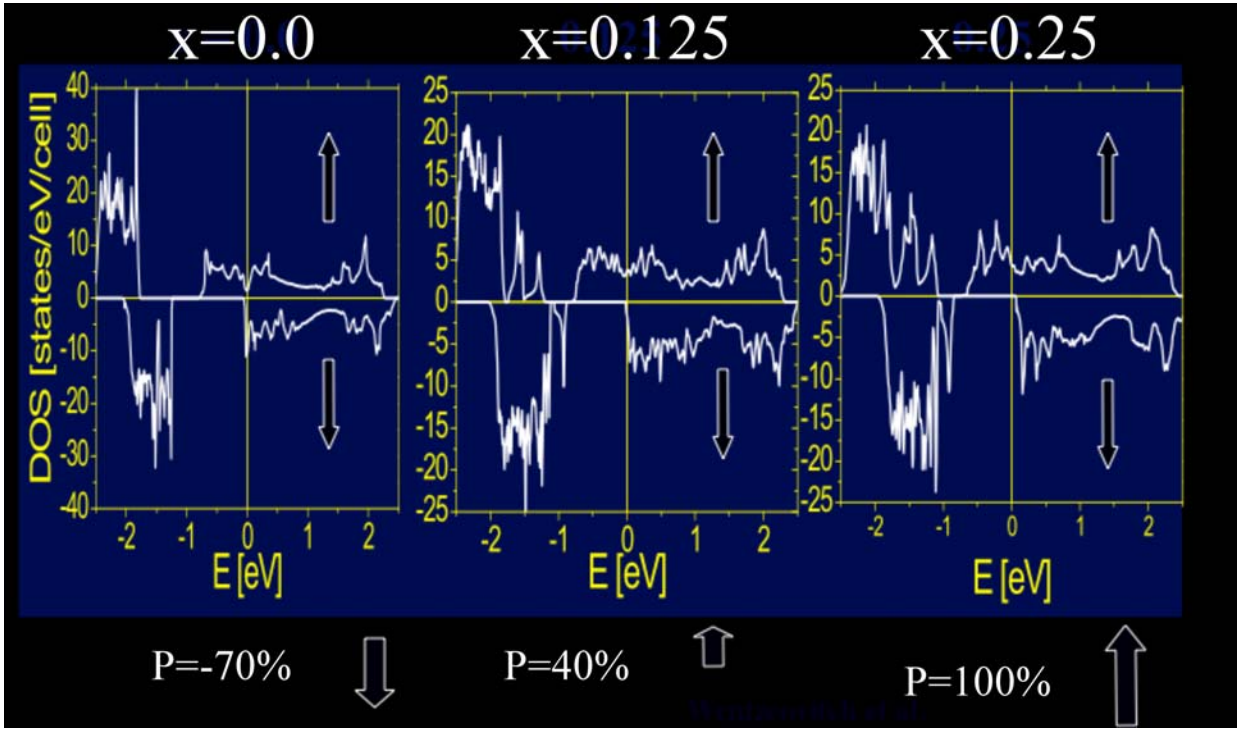
Institute for the Theory of Advanced Materials in Information Technology: James R. Chelikowsky, Yousef Saad and Renata Wentzcovitch (Minnesota), Steven G. Louie (UC Berkeley) and Efthimios Kaxiras (Harvard) (DMR-0325218): Spintronic Materials



Density of states for $Co_{1-x}Fe_xS_2$. The Fermi-level is taken as the energy zero. For x=0, the material is a ferromagnetic metal with "negative" spin polarization as the minority electrons predominate at the Fermi level. The predicted change in sign of the polarization as a function of x has been experimentally confirmed.

Spintronic materials are designed to have large spin polarization at the Fermi-level. We have been examining alloys such as $Co_{1-x}Fe_xS_2$.
CoS_2 is a metallic ferromagnet, FeS_2 is a diamagnetic semiconductor. By alloying the two sulfides we can change the net polarization:

$$P = \frac{n_\uparrow - n_\downarrow}{n_\uparrow + n_\downarrow}$$

Our goal is to produce a half-metallic material, i.e., P=1.

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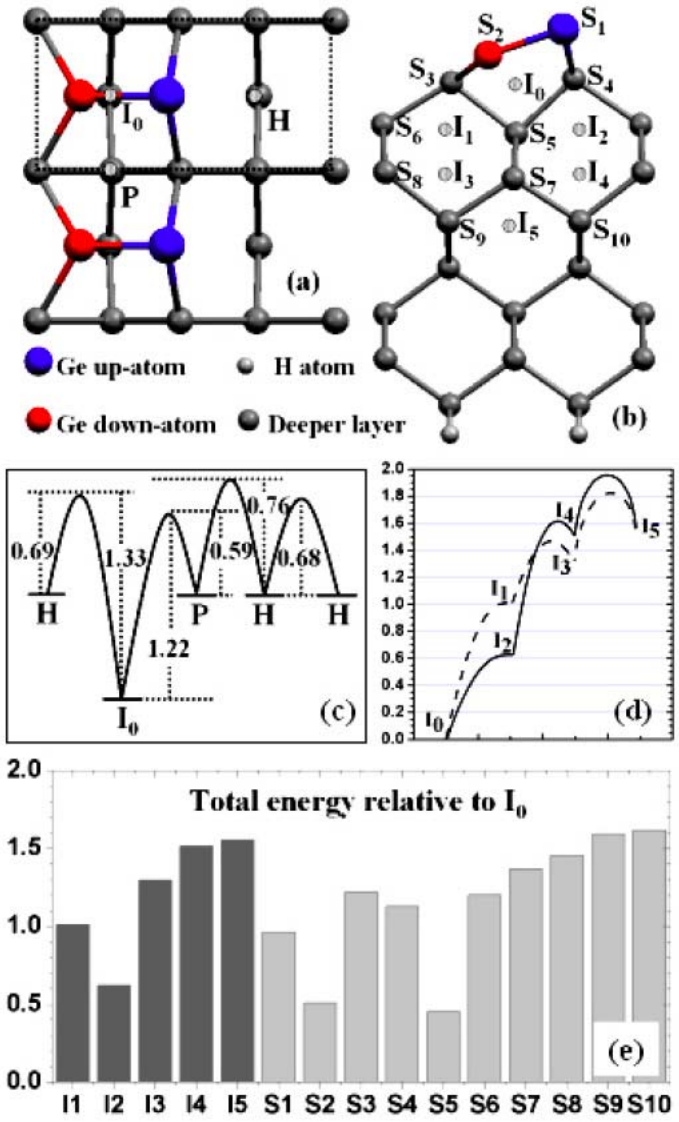
Understanding growth mechanisms of spintronics materials such as Mn:Ge is an important, but largely unexplored issue. We use pseudopotential-density functional theory to examine the growth of Mn on Ge surfaces. We find that low Mn doses on Ge (100) surface initiates novel subsurface growth whereas Mn on the (111) surface can diffuse into the bulk via interstitial sites. On the right, we show various positions of Mn on the (100) Ge surface. All the sites are less energetically favorable than the interstitial site (I_o). As such, thermodynamic considerations suggest that Mn will always reside just beneath the Ge surface.



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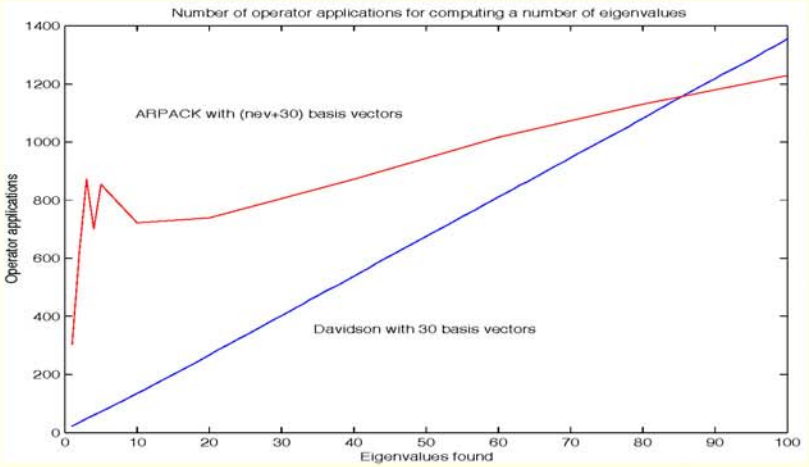
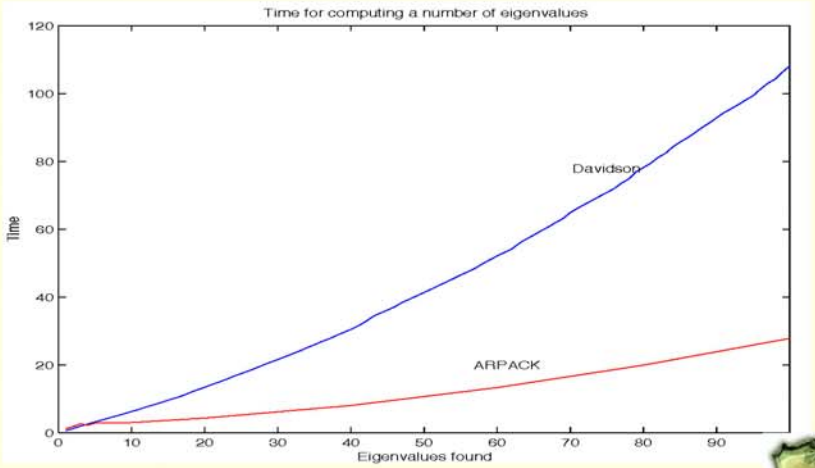
Electronic structure calculations often require the solution of an eigenvalue problem, sometimes involving hundres, if not thousands of eigenvalues. A commonly used method by our group is the generalized Davidson method. This method often uses powerful preconditioners to obtain the required solution. We have been investigating alternate methods such as ARPACK, which does not use preconditioners. We found for many cases that ARPACK is a faster method, although it requires more numerical operations.





From Andreas Stathopoulos

FFT-based methods for Time-Dependent Density Functional Theory (TDDFT)

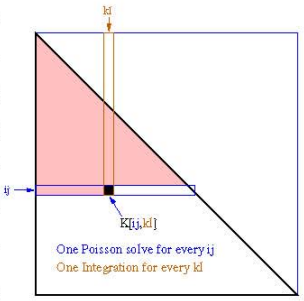
Jim Chelikowsky (PI) and Yousef Saad – NSF DMR-0325218

Background. Time-Dependent Density Functional Theory methods are used for studying excited state properties which cannot be obtained by standard DFT. We employ a method based on a frequency space representation. In this technique a large coupling matrix K is to be computed, and this constitutes a major computation when the number of atoms increases. Starting in 1999, our group implemented an initial parallel code which enabled the largest TDDFT computation at that time.

New Approach. Later the same code was optimized with the help of the Computer Science team achieving a factor of about 5 gain in execution time as well as substantial gains in memory usage. Recently, we moved to a new method which exploits FFT to solve the linear systems arising in the construction of K. The initial computational time went from a few days, to 15 hours, to 1.5 hours (most recent result).

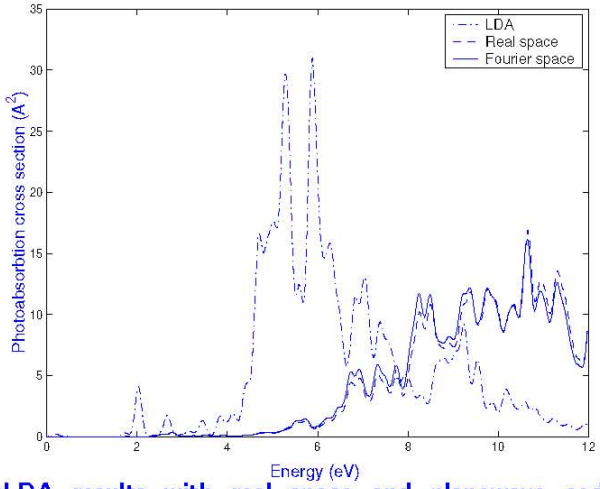
Results. The table shows wall-clock time of the parallel TDLDA code using Fourier space and Real Space for the Si34H36 test case running on 8 processors

Method	Wall-Clock Time (hours)
Real Space Code	15:30
PW: Initial Implementation	3:30
PW: Optimized load balancing	1:30



Coupling Matrix K

Each row of the coupling matrix requires solving a Poisson Equation which translate into a (sparse) linear system on the whole domain. Our initial approach used Conjugate Gradient. The new approach exploits the FFT and knowldge about the decay of the wavefunctions to solve these systems efficiently.



TDLDA results with real space and planewave codes ($Si34H36$). Also shown are results obtained with LDA.

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The Institute for the Theory of Advanced Materials in Information Technology organized a joint meeting between US researchers and their European counterparts. The meeting was held at the behest of the Division of Materials Research of the National Science Foundation and the European Commission on methods in computational materials science. The goal of the workshop was to explore and assess current opportunities in computational materials science. New computational methods for understanding and predicting materials properties and phenomena will be examined. Of particular interest were those properties and phenomena that span multiple time and length scales and require multiscale modeling to compute the essential science.

The meeting was held during the week of the spring meeting of the Materials Research Society on April 15 and 16, 2004.

The report of the meetging can be found on the website: http://www-itamit-test.dtc.umn.edu/nsfreport.php

Esteban Busso (above). Imperial College, UK, co-organized the meeting with Jim Chelikowsky, University of Minnesota.

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The Institute for the Theory of Advanced Materials in Information Technology hosted a meeting at the Digital Technology Center on the campus of the University of Minnesota on August 6 and 7, 2004. The meeting focused on an assessment of the important materials problems in information technology. International scientists from Portugal, Italy, Germany and Israel and industrial scientists from Intel, Texas Instruments and 3M made presentations. Many of these presentations can be found at the website:

http://www.itamit.dtc.umn.edu/meeting.html

Steve Louie (UC Berkeley), Y.K. Kwon (Minnesota) and Gaddi Haase (Texas Instruments)

Jim Chelikowsky (Minnesota), Steve Louie (UC Berkeley) and Jose Martins (INESC Lisbon)

Institute for the Theory of Advanced Materials in Information Technology: James R. Chelikowsky, Yousef Saad and Renata Wentzcovitch (Minnesota), Steve Louie (UC Berkeley) and Efthimios Kaxiras (Harvard) (DMR-0325218): Education and Training

Educational:
5 grad students
5 post-docs
2 undergraduat interns
Training centers on computational materials science, physics, chemical physics, scientific computation and computer science. Current research projects include magnetic semiconductors, semiconductor liquids, clusters, quantum dots and high performance, scalable algorithms for materials problems.

Outreach:
Web site for the distribution of computer codes and computational materials science. Coordination meeting with International and International Advisory Boards.

Graduate Students at Minnesota (left to right). Shiv Gowda, Lingzhu Kong, Shen Li and Marie Lopez del Puerto

Summer interm program:
Program established with the Minnesota Supercomputing Institute. First intern: **Eric Lindgren** from Carlton College. Eric worked on III-V semiconductor quantum dots.